

# Schrödinger Equation for Heavy Mesons Expanded in $1/m_Q$

Takayuki Matsuki \*

*Tokyo Kasei University, 1-18-1 Kaga, Itabashi, Tokyo 173, JAPAN*

## Abstract

Operating just once the naive Foldy-Wouthuysen-Tani transformation on the Schrödinger equation for  $Q\bar{q}$  bound states described by a hamiltonian, we systematically develop a perturbation theory in  $1/m_Q$  which enables one to solve the Schrödinger equation to obtain masses and wave functions of the bound states in any order of  $1/m_Q$ . It is shown that positive energy projection with respect to the heavy quark sector of a wave function is, at each order of perturbation, proportional to the 0-th order solution. There appear also negative components of the wave function except for the 0-th order, which contribute also to higher order corrections to masses.

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\*E-mail: matsuki@tokyo-kasei.ac.jp or matsuki@ins.u-tokyo.ac.jp

## I. INTRODUCTION

Since the introduction of the ingenious notion of heavy quark effective theory (HQET),<sup>1</sup> many physical quantities, especially regarding to  $B$  mesons, have been calculated. Furthermore formulation has also been polished to incorporate higher orders.<sup>2</sup> However, the way to incorporate higher order terms is somewhat insufficient since only the operator product forms in higher orders are obtained but their matrix elements are just parameters and must be determined so that the physical quantities are fitted with experiments.<sup>3</sup> Another obscure point of HQET is that the residual momentum, which is a difference between a meson momentum and a heavy quark momentum, necessarily comes in and we do not know how properly this quantity can be taken into account as a perturbation. On this point HQET is different from QED in the sense that the next order perturbation terms cannot be determined automatically from the lower orders.

Let us remind how HQET has been constructed to calculate physical quantities regarding heavy mesons/baryons. When HQET was originally developed, lagrangian formulation was adopted and light/heavy quarks are treated as elementary fields. In this approach an appropriate transformation only on heavy quarks is introduced so that heavy quark fields are separated into positive/negative components in energy. This picture was intuitively believed to realize the situation that a positive component of a heavy quark behaves like a static color source and a light anti-quark with gluon clouds is relativistically hanging around it, which owes most of the messy part of the strong interactions. To stress even more this intuitive idea, one assumes that a heavy quark carries most of the momentum of a heavy meson, which yields a residual momentum.

Even though the above formulation has been well developed, this cannot be applied straightforwardly to the Schrödinger equation for a bound state of a  $Q\bar{q}$  system. It is the purpose of this paper to construct a perturbation theory in  $1/m_Q$  *a la* HQET for a hamiltonian system, i.e., for a bound system which is described by a hamiltonian with an appropriate potential. Instead of particle fields, wave functions of a  $Q\bar{q}$  system *at rest*

are the objects to deal with. Then matrix elements of currents/operators between heavy mesons are calculable at any order in principle since meson wave functions are calculated as solutions to the Schrödinger equation together with their masses as eigenvalues with corrections and there appears no residual momentum of a heavy quark in this formulation. In our formulation, at first the naive Foldy- Wouthuysen-Tani (FWT)<sup>4</sup> transformation is introduced and instead of working only with positive components of heavy quark fields there appear negative components as well and hence the formulae to calculate those negative components are also given at each order of perturbation. This formulation gives different results from the previous calculations<sup>5</sup> on the masses of  $D$ ,  $D^*$ ,  $B$  and  $B^*$  because of negative components of heavy quark sector which is briefly mentioned at the end of this letter.

## II. HAMILTONIAN

A projection operator which extracts a positive component of a heavy quark plays an important role in HQET. In a much more precise statement this projection operator is defined so that the equation for the two upper components of a Dirac spinor (positive components) does not mix with the two lower components (negative components) in the lagrangian. Here before introducing a projection operator, let us recall what the naive FWT transformation does. This transformation, when it operates on a free Dirac Schrödinger equation, turns a kinematic hamiltonian,  $\vec{\alpha} \cdot \vec{p} + m\beta$ , into  $E\beta$  and leaves us only the two upper components of a free wave function.

$$U_{FWT} (\vec{\alpha} \cdot \vec{p} + m\beta) U_{FWT}^{-1} U_{FWT}\phi = E U_{FWT}\phi \quad \rightarrow \quad E \beta U_{FWT}\phi = E U_{FWT}\phi,$$

i.e.,

$$E (1 - \beta) U_{FWT}\phi = 0,$$

which means that  $(1 + \beta)/2 U_{FWT}\phi = U_{FWT}\phi$ , i.e., only the two upper components of  $U_{FWT}\phi$  survive. Here

$$U_{FWT}(p) = \exp(W(p) \vec{\gamma} \cdot \vec{n}) = \cos W + \vec{\gamma} \cdot \vec{n} \sin W, \quad (1)$$

$$\vec{n} = \frac{\vec{p}}{p}, \quad \tan W(p) = \frac{p}{m + E}. \quad (2)$$

As one can see, in this formulation a projection operator,  $(1 - \beta)/2$ , naturally comes in to exclude two lower components. Based on this fact, introduction of the FWT transformation may give us a good starting point for studying a  $Q\bar{q}$  system as in fact will be seen later rather than trying to develop a perturbation theory of the original hamiltonian without any transformation.

The state of a bound state in this paper is defined by

$$|\psi\rangle = \int d^3x \int d^3y \psi_{\alpha\beta}(x - y) q_{\alpha}^c{}^{\dagger}(x) Q_{\beta}^{\dagger}(y) |0\rangle, \quad (3)$$

where  $q^c$  is a charge conjugate field of a light quark  $q$  and its conjugate state by  $\langle\psi| = |\psi\rangle^{\dagger}$  with  $\langle 0| \equiv |0\rangle^{\dagger}$ . Given a hamiltonian density,  $\mathcal{H}$ , for a  $Q\bar{q}$  system, varying the quantity

$$\langle\psi| (\mathcal{H} - E) |\psi\rangle,$$

in terms of  $\psi_{\alpha\beta}(x - y)$ , and setting it equal to zero, then we have the matrix form of the Schrödinger equation

$$H \psi = (m_Q + \tilde{E}) \psi.$$

Here a bound state mass  $E$  is broken into two parts,  $m_Q$  and the rest,  $\tilde{E}$ . A binding energy is given by  $\tilde{E} - m_Q$ . Operating the FWT transformation only on a heavy quark sector in this equation at the center of the mass system of a bound state, one can modify the Schrödinger equation as,

$$(H_{FWT} - m_Q) \psi_{FWT} = \tilde{E} \psi_{FWT}, \quad (4)$$

where

$$H_{FWT} = U_{FWT}(p'_Q) H U_{FWT}^{-1}(p_Q), \quad \psi_{FWT} = U_{FWT}(p_Q) \psi. \quad (5)$$

Note that the argument of the FWT transformation operated on a hamiltonian from left is different from the right-operated one, since an outgoing momentum,  $\vec{p}_Q'$ , are different from

incoming one,  $\vec{p}_Q$ . Expressing model-dependent instantaneous potential terms as  $H^{int}$ , a hamiltonian is given by

$$H = \vec{\alpha}_q \cdot \vec{p}_q + m_q \beta_q + \vec{\alpha}_Q \cdot \vec{p}_Q + m_Q \beta_Q + H^{int}. \quad (6)$$

Next  $H_{FWT} - m_Q$  can be expanded in  $1/m_Q$ , which is given by

$$H_{FWT} - m_Q = H_{-1} + H_0 + H_1 + H_2 + \cdots, \quad (7)$$

where

$$H_{-1} = m_Q (\beta_Q - 1), \quad (8a)$$

$$H_0 = \vec{\alpha}_q \cdot \vec{p} + m_q \beta_q + H_{FWT0}^{int}, \quad (8b)$$

$$H_1 = \frac{1}{2m_Q} \vec{p}^2 \beta_Q + H_{FWT1}^{int}, \quad (8c)$$

$$H_2 = H_{FWT2}^{int}, \quad (8d)$$

$\vdots$

Here  $H_i$  stands for the  $i$ -th order hamiltonian,  $H_{FWTi}^{int}$  for the  $i$ -th order of the interaction terms and since a bound state is at rest,

$$\vec{p} = \vec{p}_q = -\vec{p}_Q, \quad \vec{p}' = \vec{p}_q' = -\vec{p}_Q', \quad \vec{q} = \vec{p}' - \vec{p},$$

are defined, where primed quantities are final momenta.

### III. PERTURBATION

Using the hamiltonian obtained in the last section, we show in this section that the Schrödinger equation can be solved order by order in  $1/m_Q$  utilizing a projection operator. First we introduce projection operators:

$$\Lambda_{\pm} = \frac{1 \pm \beta_Q}{2}, \quad (9)$$

which correspond to positive-/negative-energy projection operators for a heavy quark sector at the rest frame of a bound state. These are given by  $(1 \pm \not{v})/2$  in the moving frame of a

bound state with  $v^\mu = P^\mu/E$  in HQET where  $P^\mu$  is the four-momentum of a bound state. Then we expand the mass and wave function of a bound state in  $1/m_Q$  as

$$\tilde{E} = E_0^k + E_1^k + E_2^k + \dots, \quad (10)$$

$$\psi_{FWT} = \psi_0^k + \psi_1^k + \psi_2^k + \dots, \quad (11)$$

where  $k$  stands for a set of quantum numbers that distinguish independent eigenfunctions of the lowest order Schrödinger equation, and a subscript  $i$  of  $E_i^k$  and  $\psi_i^k$  for the order of  $1/m_Q$ .

### A. -1st order

From eqs.(4) and (8a), the -1st order Schrödinger equation in  $1/m_Q$  is given by

$$-2m_Q\Lambda_-\psi_0^k = 0, \quad (12)$$

which means

$$\psi_0^k = \Lambda_+\psi_0^k. \quad (13)$$

That is, the 0-th order wave function has only a positive component of the heavy quark sector whose form is given below.

### B. 0-th order

The 0-th order equation is given by

$$-2m_Q\Lambda_-\psi_1^k + H_0\psi_0^k = E_0^k\psi_0^k. \quad (14)$$

Multiplying projection operators,  $\Lambda_\pm$ , from left, respectively, we obtain

$$\Lambda_+H_0\psi_0^k = E_0^k\psi_0^k, \quad (15)$$

$$-2m_Q\Lambda_-\psi_1^k + \Lambda_-H_0\psi_0^k = 0. \quad (16)$$

Eq. (15) gives the lowest non-trivial Schrödinger equation. Let us assume this equation is solved<sup>6</sup> and all the independent eigenfunctions and eigenvalues are obtained analytically and/or numerically as  $E_0^k$  and

$$\psi_0^k = \Phi_k^+ = \begin{pmatrix} u_k(\vec{r}, \Omega) & 0 \\ v_k(\vec{r}, \Omega) & 0 \end{pmatrix}, \quad (17)$$

where  $u_k$  and  $v_k$  are 2 by 2 matrices. Likewise we can in general assume that a  $\Lambda_-$  component of any wave function is expanded in terms of

$$\Phi_k^- = \begin{pmatrix} 0 & u_k(\vec{r}, \Omega) \\ 0 & v_k(\vec{r}, \Omega) \end{pmatrix}. \quad (18)$$

Expanding  $\Lambda_- \psi_1^k$  in terms of this set of eigenfunctions, one can solve Eq. (16) as follows.

Setting

$$\Lambda_- \psi_1^k = \sum_{\ell} c_{1-}^{\ell k} \Phi_{\ell}^-, \quad (19)$$

one obtains coefficients,  $c_{1-}^{\ell k}$ , as

$$c_{1-}^{\ell k} = \frac{1}{2m_Q} \int r^2 dr d\Omega \operatorname{tr} \left( \Phi_{\ell}^{-\dagger} \Lambda_- H_0 \Lambda_+ \Phi_k^+ \right), \quad (20)$$

where the 0-th order wave function is normalized to be 1,

$$\int d^3r \operatorname{tr} \left( \Phi_k^{\pm \dagger} \Phi_{\ell}^{\pm} \right) = \delta_{k\ell}. \quad (21)$$

### C. 1st order

The 1st order equation is given by

$$-2m_Q \Lambda_- \psi_2^k + H_0 \psi_1^k + H_1 \psi_0^k = E_0^k \psi_1^k + E_1^k \psi_0^k. \quad (22)$$

As in the above case, multiplying projection operators, we obtain

$$\Lambda_+ H_0 \psi_1^k + \Lambda_+ H_1 \psi_0^k = E_0^k \Lambda_+ \psi_1^k + E_1^k \psi_0^k, \quad (23)$$

$$-2m_Q \Lambda_- \psi_2^k + \Lambda_- H_0 \psi_1^k + \Lambda_- H_1 \psi_0^k = E_0^k \Lambda_- \psi_1^k. \quad (24)$$

When one looks at Eq. (23), one easily notices that this can be separated into two independent equations. One equation gives a solution to the positive component of  $\psi_1^k$  as

$$\Lambda_+ H_0 \Lambda_+ \psi_1^k = E_0^k \Lambda_+ \psi_1^k,$$

which means from Eq. (15) that

$$\Lambda_+ \psi_1^k = c_{1+}^k \Phi_k^+, \quad (25)$$

and the coefficient,  $c_{1+}^k$ , should be determined by a normalization of the wave function up to the first order,

$$\int d^3r \operatorname{tr} (\psi^{k\dagger} \psi^k) = 1, \quad (26)$$

whose definition is allowed because here we are not calculating the absolute value of the form factors. The appropriate normalization will be determined in future papers in which we will give several kinds of form factors. Using this equation, one easily notices that up to the first order,

$$c_{1+}^k = 0, \quad (27)$$

where the coefficient is assumed to be real. This completes the solution for  $\psi_1^k$  since  $\Lambda_- \psi_1^k$  is obtained in the last chapter, i.e.,

$$\psi_1^k = \sum_{\ell} c_{1-}^{\ell k} \Phi_{\ell}^-. \quad (28)$$

Another equation is given by

$$\Lambda_+ H_0 \Lambda_- \psi_1^k + \Lambda_+ H_1 \psi_0^k = E_1^k \psi_0^k, \quad (29)$$

which gives the first order perturbation corrections to the mass when one calculates matrix elements of the lhs among eigenfunctions,  $\Phi_k^{\pm}$  like in the ordinary perturbation of quantum mechanics.

Eq. (24) gives a  $\Lambda_-$  component of  $\psi_2^k$  as in the case of  $\Lambda_- \psi_1^k$  in subsection IIIB, i.e., setting



$$\Lambda_- \psi_2^k = \sum_{\ell} c_{2-}^{\ell k} \Phi_{\ell}^-, \quad (30)$$

one obtains coefficients,  $c_{2-}^{\ell k}$ , as

$$c_{2-}^{\ell k} = \frac{1}{2m_Q} \int r^2 dr d\Omega \operatorname{tr} \left[ \Phi_{\ell}^{-\dagger} \left( \Lambda_- H_0 \psi_1^k + \Lambda_- H_1 \Phi_k^+ - E_0^k \Lambda_- \psi_1^k \right) \right]. \quad (31)$$

#### D. 2nd order

The 2nd order equation is given by

$$-2m_Q \Lambda_- \psi_3^k + H_0 \psi_2^k + H_1 \psi_1^k + H_2 \psi_0^k = E_0^k \psi_2^k + E_1^k \psi_1^k + E_2^k \psi_0^k. \quad (32)$$

As in the above cases, multiplying projection operators, we obtain

$$\Lambda_+ H_0 \psi_2^k + \Lambda_+ H_1 \psi_1^k + \Lambda_+ H_2 \psi_0^k = E_0^k \Lambda_+ \psi_2^k + E_1^k \Lambda_+ \psi_1^k + E_2^k \Lambda_+ \psi_0^k, \quad (33)$$

$$-2m_Q \Lambda_- \psi_3^k + \Lambda_- H_0 \psi_2^k + \Lambda_- H_1 \psi_1^k + \Lambda_- H_2 \psi_0^k = E_0^k \Lambda_- \psi_2^k + E_1^k \Lambda_- \psi_1^k. \quad (34)$$

When one looks at Eq. (33), one easily notices that this can be separated into three independent equations. The first one gives a solution to the positive component of  $\psi_2^k$ :

$$\Lambda_+ H_0 \Lambda_+ \psi_2^k = E_0^k \Lambda_+ \psi_2^k,$$

which means from Eq. (15) that

$$\Lambda_+ \psi_2^k = c_{2+}^k \Phi_k^+. \quad (35)$$

The coefficient,  $c_{2+}^k$ , should be determined by a normalization of the wave function up to the second order using Eq. (26) and by assuming the coefficient is real, it is given by

$$c_{2+}^k = -\frac{1}{2} \left( \sum_{\ell} c_{1-}^{\ell k} \right)^2. \quad (36)$$

There are some other contributions to this coefficient,  $c_{2+}^k$ , from transitions of  $\Phi_k^+$  to other states and back to  $\Phi_k^+$  which are obtained when one diagonalizes the whole energy matrix. This completes the solution for  $\psi_2^k$  when combined with the  $\Lambda_-$  component obtained above.

$$\psi_2^k = c_{2+}^k \Phi_k^+ + \sum_{\ell} c_{2-}^{\ell k} \Phi_{\ell}^-. \quad (37)$$

The second equation is given by

$$a\Lambda_+H_1\Lambda_-\psi_1^k + \Lambda_+H_1\Lambda_+\psi_1^k = E_1^k\Lambda_+\psi_1^k,$$

where  $a$  is determined so that this equation coincides with the first order energy correction equation, Eq. (29), using  $\Lambda_+\psi_1^k = c_{1+}^k\psi_0^k$ :

$$a = c_{1+}^k = 0.$$

The third equation is given by the remainder,

$$\Lambda_+H_0\Lambda_-\psi_2^k + \Lambda_+H_1\Lambda_-\psi_1^k + \Lambda_+H_2\psi_0^k = E_2^k\Lambda_+\psi_0^k, \quad (38)$$

which gives the second order corrections to the energy by taking the matrix elements of the lhs among  $\Phi_k^{\pm}$ .

Eq. (34) gives a  $\Lambda_-$  component of  $\psi_3^k$  as in the cases of  $\Lambda_-\psi_1^k$  and  $\Lambda_-\psi_2^k$  given in subsections IIIB and IIIC, i.e., setting

$$\Lambda_-\psi_3^k = \sum_{\ell} c_{3-}^{\ell k} \Phi_{\ell}^-, \quad (39)$$

one obtains coefficients,  $c_{3-}^{\ell k}$ , as

$$c_{3-}^{\ell k} = \frac{1}{2m_Q} \int r^2 dr d\Omega \operatorname{tr} \left[ \Phi_{\ell}^{-\dagger} \left( \Lambda_-H_0\psi_2^k + \Lambda_-H_1\psi_1^k + \Lambda_-H_2\Phi_k^+ - E_0^k\Lambda_-\psi_2^k - E_1^k\Lambda_-\psi_1^k \right) \right]. \quad (40)$$

## E. Higher order

The  $i$ -th order equation is given by

$$-2m_Q\Lambda_-\psi_{i+1}^k + \sum_{j=0}^i H_j\psi_{i-j}^k = \sum_{j=0}^i E_j^k\psi_{i-j}^k. \quad (41)$$

We follow the previous subsections to derive all the results from this equation below. Multiplying projection operators, we obtain

$$\sum_{j=0}^i \Lambda_+ H_j \psi_{i-j}^k = \sum_{j=0}^i E_j^k \Lambda_+ \psi_{i-j}^k, \quad (42)$$

$$-2m_Q \Lambda_- \psi_{i+1}^k + \sum_{j=0}^i \Lambda_- H_j \psi_{i-j}^k = \sum_{j=0}^{i-1} E_j^k \Lambda_- \psi_{i-j}^k. \quad (43)$$

Eq. (42) gives a solution to a positive component of  $\psi_i^k$  as

$$\Lambda_+ H_0 \Lambda_+ \psi_i^k = E_0^k \Lambda_+ \psi_i^k, \quad (44)$$

which means

$$\Lambda_+ \psi_i^k = c_{i+}^k \Phi_k^+, \quad (45)$$

where the coefficient,  $c_{i+}^k$ , should be determined by a normalization of the wave function, Eq. (26), up to the  $i$ -th order and there are of course other contributions mentioned in subsection III D. This completes the solution for  $\psi_i^k$  when combined with the  $\Lambda_-$  component obtained from the  $(i-1)$ -th order equation. Eq. (42) also includes other equations, which are identified as the  $(i-j)$ -th order ( $j = 1 \sim i-1$ ) energy correction equations. These are straightforwardly obtained order by order though complicated and hence are omitted here. After extracting these equations, the remainder of Eq. (42) gives the  $i$ -th order energy correction equation. Eq. (43) gives a  $\Lambda_-$  component of  $\psi_{i+1}^k$ , i.e., setting

$$\Lambda_- \psi_{i+1}^k = \sum_{\ell} c_{i+1,-}^{\ell k} \Phi_{\ell}^-, \quad (46)$$

one obtains coefficients,  $c_{i+1,-}^{\ell k}$ , as

$$c_{i+1,-}^{\ell k} = \frac{1}{2m_Q} \int r^2 dr d\Omega \operatorname{tr} \left[ \Phi_{\ell}^{-\dagger} \left( \sum_{j=0}^{i-1} \Lambda_- (H_j - E_j^k) \psi_{i-j}^k + \Lambda_- H_i \Phi_k^+ \right) \right], \quad (47)$$

where all the  $E_j^k$  are the values obtained by diagonalizing the lhs of the  $j$ -th order energy correction equation.

#### IV. CONCLUSIONS

In this letter we have developed a systematic perturbation of the Schrödinger equation for a bound state of  $Q\bar{q}$  at rest in  $1/m_Q$  by using just once the naive Foldy-Wouthuysen-Tani

transformation on the heavy quark sector. The effects of the FWT transformation is, as can be seen from Eq. (8), to treat the heavy quark as a non-relativistic color source. It is shown that all the positive components of wave functions at each order of perturbation are proportional to the lowest order solution,  $\Phi_k^+$  except that  $c_{1+}^k = 0$ . There also appear negative components of wave functions for heavy quark sector, which can also be perturbatively solved. As one can easily notice, the lowest order equation, Eq. (15), can be derived by any method. That is, we do not need to introduce the FWT or any other transformation to obtain this equation. The higher order terms in  $1/m_Q$ , however, reflect what kind of transformation is introduced and we believe that any transformation which utilizes the properties of a heavy quark will give a better perturbation as has been shown by HQET than that without a transformation.

To make formulae simple in this letter, all the gamma matrices of light and heavy quarks are multiplied from left with the wave function,  $\psi^k$ . To make the wave function a true bispinor, the Schrödinger equation should be transformed by a charge conjugation operator  $U_c = i\gamma_Q^0\gamma_Q^2$  for a heavy quark. That is,  $U_c\psi^k$  becomes a bispinor,  $U_c H_{FWT} U_c^\dagger$  is a hamiltonian of interest, and gamma matrices of a light anti-quark is multiplied from left while those of a heavy quark from right.

One example for model dependent interaction terms is, e.g., given by<sup>5,7</sup>

$$\beta_q\beta_Q S(r) + \left\{1 - \frac{1}{2}[\vec{\alpha}_q \cdot \vec{\alpha}_Q + (\vec{\alpha}_q \cdot \vec{n})(\vec{\alpha}_Q \cdot \vec{n})]\right\} V(r), \quad (48)$$

where  $\vec{n} = \vec{r}/r$ . This model is being studied by using our formulation, in which masses and eigenfunctions of  $D$ ,  $D^*$ ,  $B$  and  $B^*$  are calculated including all those corrections mentioned in Sec.III and spin-flavor symmetry at the lowest order is realized by a special quantum number related to the heavy quark spin.<sup>6</sup> Our formulation gives the same results as those in<sup>5</sup> if negative components are neglected and if only the terms up to  $1/m_Q^2$  in the hamiltonian are taken into account.

In order to calculate, e.g., the semileptonic weak decay  $B \rightarrow D + \ell\nu$ , one needs to boost the  $D$  meson even if the  $B$  meson is at rest. The formulation obtained in this letter does

not give any prescription how to construct a boosted wave function. We will propose some method in a future paper to compute the form factors by using wave functions calculated by the method proposed in this letter.

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